FEMSTER: An object oriented class library of discrete differential forms

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1   Introduction

The equations of electromagnetics can be simply and elegantly cast in the language of differential geometry, more precisely in terms of differential forms or p-forms [1], [2], [3]. In this geometrical setting, the fundamental conservation laws are not obscured by the details of coordinate system dependent notation; and, the governing equations can be reformulated in a more compact and clear way using well known differential operators of the exterior algebra such as the exterior derivative, the wedge product, and the Hodge star operator. In this context, a natural framework for the modeling of physical quantities is also provided. For example, the electric potentials can be represented by 0-forms; electric and magnetic fields by 1-forms; electric and magnetic fluxes by 2-forms; and, scalar charge density by 3-forms.

Our primary motivation for the development of FEMSTER was the need for a common finite element framework for electrostatics, magnetostatics, eddy current problems, Helmholtz equation, time-dependent Maxwell equations, etc. Recently, Hiptmair [4], motivated by the theory of exterior algebra of differential forms, presented a unified mathematical framework for the construction of conforming finite element spaces. Remarkably, both $\mathcal{H}(curl)$ and $\mathcal{H}(div)$ conforming finite element spaces and the definition of their degrees of freedom and interpolation operators can be derived within this framework. Given a physical law expressed in the language of differential forms, it is quite straightforward to discretize the problem using our class library. Our second motivation was the need for high-order discretization which can reduce the mesh size, memory usage, and CPU time required to achieve a prescribed error tolerance. This is particularly true for electrically large problems due to numerical dispersion. The FEMSTER library contains implementations of finite element basis functions of arbitrary order. These implementations include both uniform and non-uniform interpolatory bases, the latter providing significantly improved numerical stability as the order is increased.

2   PDE's and exterior algebras

We begin with the generic boundary value problem stated in the language of differential forms from [5]. We assume a 3-dimensional domain Ω with piecewise smooth boundary $\partial\Omega$ partitioned into Γ_D, Γ_N, and Γ_M. The problem statement is

$$du = (-1)^p\sigma, \;\; dj = -\Psi + \Phi, \; j = \star_\alpha \sigma, \;\; \Psi = \star_\gamma u \; in \;\; \Omega \tag{1}$$

$$T_D u = f \ \ on \ \ \Gamma_D, \ \ T_N j = g \ \ on \ \ \Gamma_N, \ \ T_M j = (-1)^p \star^\beta \ T_M u \ \ on \ \ \Gamma_M. \tag{2}$$

Here u is a $(p-1)$-form, σ is a p-form, j is a $(3-p)$-form, and both Ψ and Φ are $(3-p+1)$-forms, where $1 \le p \le 3$. The variable Φ is a source term. In (1) the operator d is the exterior derivative which maps p-forms to $(p+1)$-forms. In the boundary conditions (2) the symbol T denotes the trace operator, where the trace of a p-form is an integral over a p-dimensional manifold. The $\star$ symbol denotes the Hodge-star operator, which converts p-forms to $(3-p)$-forms and typically involves material constitutive properties. Equations (1)-(2) describe, in an abstract geometrical setting, a great variety or physical problems. To be specific, when $p = 1$ we have Poisson-type problems, when $p = 2$ we have Helmholtz-type problems, and when $p = 3$ we have Stokes-like problems. The variable σ can be eliminated to yield the general second-order elliptic equation

$$(-1)^p d \star_\alpha \ du = - \star_\gamma \ u + \Phi. \tag{3}$$

A Galerkin finite element solution of the generic second-order equation (3) will require bilinear forms. Using the exterior algebra, the bilinear forms required in the Galerkin finite element method can be easily formulated from the general second-order equation (3) by taking the wedge product with an $(l-1)$-form v and integrating over the volume Ω and using the standard integration-by-parts formula. This yields the two key symmetric bilinear forms

$$a(u, v) \ = \ \int_\Omega \star_\alpha (du) \wedge dv, \tag{4}$$

$$b(u, v) \ = \ \int_\Omega \star_\gamma u \wedge v. \tag{5}$$

3   FEMSTER : a finite element class library

The philosophy of the FEMSTER library is derived from the formulation of an abstract conforming finite element method, see [6]. From the implementation point of view, such a formulation is uniquely determined by the $4-$tuple $(\Sigma, \mathcal{P}, \mathcal{A}, \mathcal{Q})$ where: Σ is a geometric element, $\mathcal{P}$ is a finite element space defined on Σ, $\mathcal{A}$ is the set of degrees of freedom defined on Σ, and $\mathcal{Q}$ is a quadrature rule defined on Σ. At the highest level, the FEMSTER library adheres closely to this well-established mathematical definition of a finite element. The four main classes are an *Element3D* class, an *IntRule3D* class, a *pForm* class, and a *BilinearForm* class.

The *pForm* class provides a common interface for all of the finite element basis functions. The class hierarchy is illustrated in Figure 3. There are derived classes for 0-forms, 1-forms, 2-forms and 3-forms. There are further specializations for the geometric elements of type *Tetrahedron, Hexahedron,* and *Prism.* Given the degree of the form and the element type, the polynomial space $\mathcal{P}$ is uniquely defined. At the lowest level of the *pForm* class hierarchy are the concrete implementations. The concrete implementations contain the specific degrees of freedom $\mathcal{A}$ of the bases, for example our Silvester-Lagrange (SL) bases are similar to the bases defined in [7] which use equidistant and shifted equidistant interpolation points. These are suitable for low order approximations, *i.e.*, $k = 1$ to 4. This particular choice of interpolation points can produce badly conditioned mass and stiffness matrices when high order approximations are used. For this reason we have implemented spectral classes that use arbitrary sets of interpolation points, typically Gauss-Lobatto or Tchebyschev points. As an example, Figure 2 shows the number of iterations required for a conjugate gradient algorithm to solve the linear system (with an error tolerance of 10^{-12}) arising from the discretization of Poisson's equation using a 0-form basis on a hexahedral mesh. In this example we show the results for three different types of interpolatory bases. The other key class is the *BilinearForm* class. Given an *Element3D*, an *IntRule3D*, and a *pForm*, the *BilinearForm* class computes the bilinear forms (4) and (5). The discrete bilinear forms are

local finite element mass and stiffness matrices, which can then be assembled to form linear systems of equations. Using these classes, the FEMSTER library provides arbitrary order discretizations of key differential operators in electromagnetics.
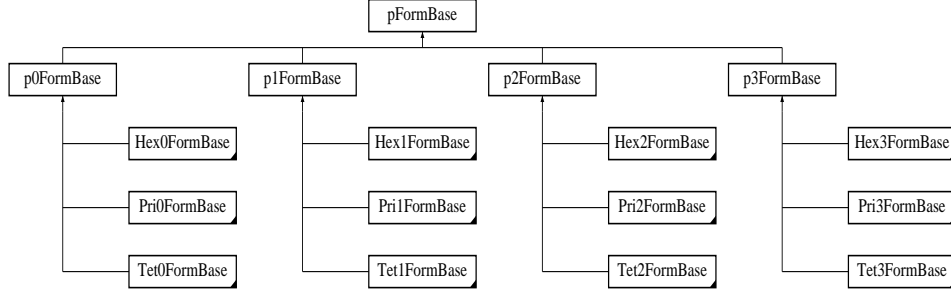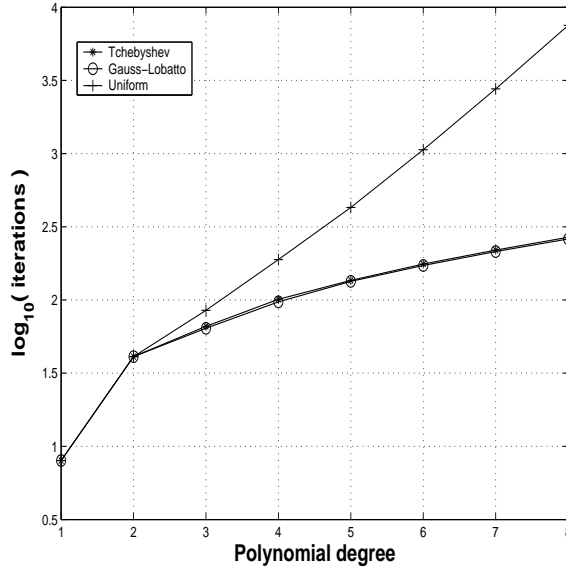

Figure 1: p-Form class inheritance

Figure 2: Iteration count for conjugate gradient solution of Poisson's equation using three different interpolatory bases, indicating improved stability of spectral degrees of freedom.

As an example of the accuracy that can be achieved using higher-order bases, we solve the vector Helmholtz equation on a sequence of tetrahedral meshes for a problem with a known, smooth solution. In Figure 3 we show the computed L_2 error versus element size h on a $\log - \log$ scale for 1-form basis functions of degree 1 through 6. The slopes of the lines (based on least-squares fit of the last three data points) are $(0.98, 1.97, 2.97, 3.97, 4.97, 5.98)$ indicating the optimal convergence. It is interesting to note that for this particular problem using a 6th order basis on a 1440 element mesh yields a solution accurate to 10 significant digits, where a comparable solution using a 1st order basis would require a mesh consisting of billions of elements.

4   Concluding remarks

The FEMSTER finite element class library described in this paper is unique in several respects. First,it is based upon the language of differential forms. This language provides a unified description of a great variety of PDE's, and thus leads us directly to a concise and
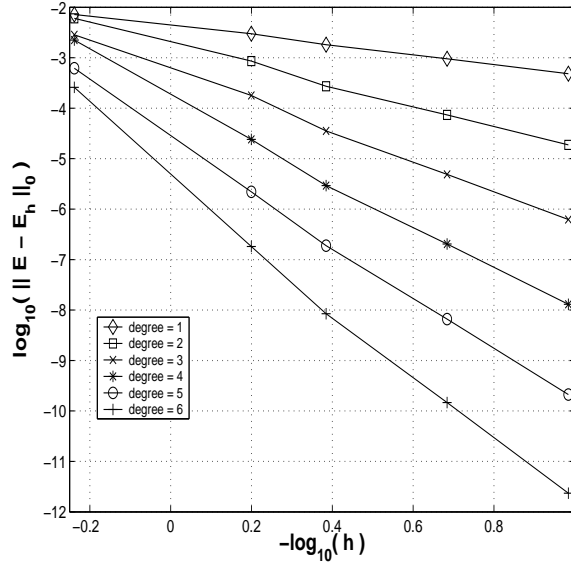
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Figure 3: Polynomial convergence of h-refined solutions of the vector Helmholtz equation using finite element 1-Form basis functions of degree 1 through 6.

abstract interface to our finite element methods. This language also unifies the seemingly disparate Lagrange, $H(curl)$ and $H(div)$ basis functions that are used in computational electromagnetics. Secondly, FEMSTER utilizes higher-order elements, bases, and integration rules. Higher-order elements are important for accurate modeling of curved surfaces. The use of higher-order basis functions reduces the demands put upon mesh generation, e.g. a billion element mesh is no longer required for a numerically converged solution. The FEMSTER class library is ideally suited for researchers who wish to experiment with unstructured-grid, higher-order solution of Poisson's equation, the Helmholtz equation, Maxwell's equations, and related PDE's that employ the standard gradient, curl, and divergence operators.

References

[1] G. Deschamps. Electromagnetics and differential forms. *IEEE Proceedings.*, 69(6):676–687, 1981.

[2] D. Baldomir. Differential forms and electromagnetism in 3-dimensional Euclidean space R3. *IEEE Proceedings.*, 133(3):139–143, 1986.

[3] A. Bossavit. *Computational Electromagnetism : variational formulation, complementarity, edge elements.* Academic Press, 1998.

[4] R. Hiptmair. Canonical construction of finite elements. *Math. Comp.*, 68(228):1325–1346, 1999.

[5] R. Hiptmair. Discrete Hodge operators: An algebraic perspective. *J. Electromagnteic Waves Appl.*, 15(3):343–344, 2001.

[6] P G. Ciarlet. *The Finite Element Method for Elliptic Problems.* North-Holland, 1978.

[7] R. Graglia, P. Wilton, and A. Peterson. Higher order interpolatory vector bases for computational electromagnetics. *IEEE Trans. Ant. Prop.*, 45(3):329–342, 1997.